MPA MaterialsMatter

October 2008

INSIDE

Division staff receives accolades

Several members of MPA have been recently recognized for their accomplishments at the Laboratory.

Clay Macomber

Marcelo Jaime

Quanxi Jia

Piotr Zelenay

Distinguished Performance Award goes to Clay Macomber

Clay Macomber (MPA-MC) is the recipient of an Individual Distinguished Performance Award. Macomber investigates reaction mechanisms and degradation pathways of solid-state materials. He used diffuse reflectance to identify a link between the optical properties of materials and their decomposition kinetics. The materials chemistry team has been able to apply his observations to the establishment of a similar correlation for a material of interest to the weapons program. For many years such a correlation has eluded researchers concerned with establishing the production variables of this material. Extension of Macomber's work to materials production will enable an optical diagnostic of the material's quality before the material is subjected to further processing. The result is a significant savings in both time and money.

Los Alamos Distinguished Performance Awards recognize individuals, small and large teams for job performance above and beyond what is normally expected. Individuals or small teams who receive Distinguished Performance Awards have made an outstanding and unique contribution that had a positive impact on LANL's programmatic efforts or status in the scientific community, required unusual creativity or dedication of the individual or team, and resulted from a level of performance substantially beyond what normally would be expected.

Jaime, Jia, Zelenay receive Women's Career Development Mentoring Awards

Marcelo Jaime, Quanxi Jia, and Piotr Zelenay are recipients of Women's Career Development Mentoring Awards.

Jaime (MPA-NHMFL) is a staff member and acting group leader, with research in the field of quantum magnetism at low temperatures and high magnetic fields. He takes the time to get to know his mentees as people and to understand their concerns and issues. He thinks deeply about the problems and issues facing his mentees and provides a steady stream of ideas, solutions and opportunities. He goes out of his way to help build the careers of his mentees through nominations for talks, seminars and workshops and visits to universities; and introductions to other scientists in the field. Vivien Zapf (MPA-NHFML) nominated him.

Jia (MPA-STC) is a Laboratory Fellow who is mentoring six postdoctoral

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From Alex's Desk

THANK YOU!
Colleagues, this is my last note from the MPA-DO desk as your Interim Division Leader. I have fully enjoyed the last 12 months. I have learned a lot working with all of you during the good and also challenging times. We have done well and I'm proud to be part of it!!! Once again thank you all for your support. I also would like to take this opportunity to thank Marcelo Jaime for the great job he has done leading the NHMFL-LANL during my tenure at MPA-DO.

Please join me in congratulating and supporting Toni Taylor as the permanent MPA Division Leader. Toni brings a great deal of leadership experience in broad programs of interest to MPA and I'm looking forward to working with her.

I'm excited to be continuing my role as the NHMFL-LANL Director. So, if you are around TA-35 and interested in seeing really big magnets and a huge generator, please stop by and I'll be honored to show you around.

Ciao,
Alex

Awards continued. . .

researchers. Jia talks to them at the beginning of their assignments to learn what he or she wants to do in the future. He teaches the postdoctoral researchers how to develop ideas and improve their writing skills for papers and proposals. He shows tremendous dedication to his work, has frequent communication with them, even when he is away at conferences, and arranges for them to give invited talks at conferences. Hongmei Luo and Guifu Zhou (both in MPA-STC) nominated him.

Zelenay (MPA-11) is the team leader for electrocatalysis. He is a leader in the fuel cell and electrocatalysis communities, making his guidance and support invaluable for postdoctoral researchers and early career scientists. His extensive background in teaching has given him superior communication skills, which enable him to convey his knowledge to early career staff and to be an effective representative of the Fuel Cell Program. He guides early career staff who are taking on responsibilities that are important for their career advancement, such as proposal writing, establishing and maintaining collaborations, and managing the work of others. Christina Johnston (MPA-11) nominated him.

The awards, given by the Women's Diversity Working Group, recognize employees who exhibit exemplary informal or formal mentoring. The award acknowledges the importance of mentoring in enabling career development, and recognizes the time, energy, and support that mentors provide to their mentees.

Modeling of plutonium matches experimental observations

The actinides and their compounds are generally found to be strongly correlated electron materials; therefore properly modeling the consequences of their many-electron interactions is challenging. Because electronic structure methods, such as the local density approximation, often fail to capture what is observed experimentally at low energies, theoretical studies of strongly correlated 3d and 4f materials have traditionally relied on many-body models to capture such physical phenomena as itinerant ferromagnetism, antiferromagnetism, heavy fermion and non-Fermi liquid behavior, and unconventional superconductivity. A similar spectrum of behavior is observed in 5f electron materials; however, novel modeling is needed because of the multiple competing interactions that appear in their energy scale hierarchy.

Cristian Batista and Jim Gubernatis (both T-11) and Tomasz

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Universal evolution dynamics in electrical generation systems

Research by Ning Li (MPA-10) reveals for the first time the logistic growth of electrical generator unit sizes for all major fuels and prime movers. This is an intrinsic feature in evolution dynamics of the power industry and a good predictor of the market life cycles of the corresponding systems.

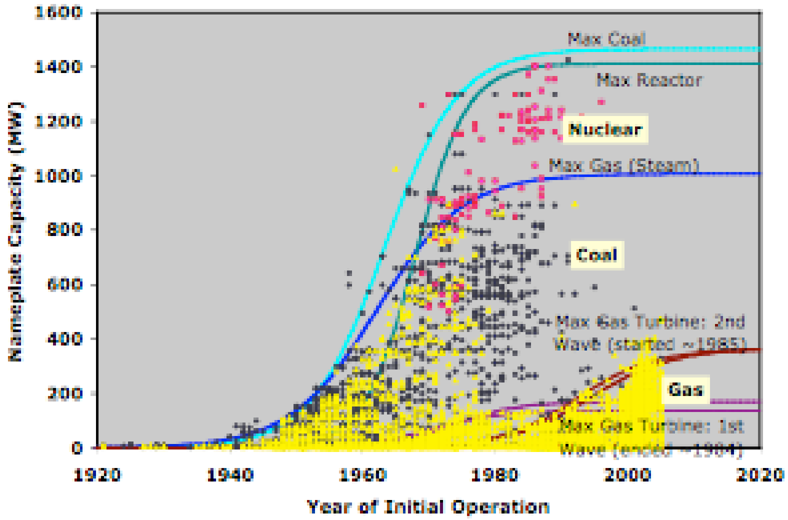

Figure illustrates the waves of growing power generation technologies (coal, gas and nuclear fueled), as indicated by the max unit-size envelopes (solid lines), and the corresponding waves of installed units (symbols) in the U.S. The (near) saturation of all major technologies, shown in the flattening of the envelopes, could indicate the need for emergence of one or two large-scale deployable technologies and systems.

Li developed a simple and elegant framework that quantitatively captures several universal dynamic features in these important, complex socio-technological systems. The analysis also predicts the need for the emergence of one or two large-scale deployable power generation technologies and systems in the next decade or so. This work provides valuable insight recommendations for the planning and resource allocation in the development of energy systems. Reference: “Size Matters: Installed maximal unit size predicts market life cycles of electricity generation technologies and systems,” *Energy Policy* **36**, 2212-2225 (2008).

Energy Policy is an international journal addressing the economic, environmental, political, planning and social aspects of energy supply and utilization that confront decision makers, corporate planners, managers, consultants, politicians and researchers. The work is funded partially through the DOE program for the Generation IV Nuclear Energy Systems.

Technical contact: Ning Li

Observations continued. . .

Durakiewicz and John Joyce (both in MPA-10) examined a strongly correlated approach to the electronic structure of actinide metals by deriving a low energy Hamiltonian H under the assumption that kinetic energy is small compared to Coulomb and spin–orbit interactions. They found that HPu for plutonium metal is similar to the effective models used for cerium and other lanthanides, but qualitatively different from the ones presented for the rest of the actinides. The researchers used HPu to calculate the photoemission spectrum and specific heat for α- and δ-plutonium and found good agreement with experiments.

This unique characteristic of plutonium metal, not seen in plutonium compounds, has important consequences for understanding the physical properties of plutonium and their relation to electronic structure. The observed f-f hopping term cancellation may be used to explain the huge volume expansion, mixed valence regime leading to lack of magnetism, and limitations of band theories that over-localize and often lead to incorrect magnetic solutions.

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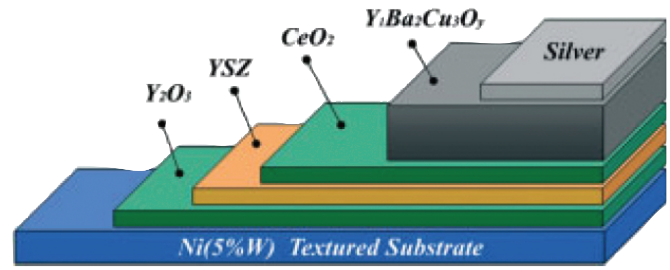
The research, “Strong Coupling Approach to Actinide Metals”, was published in *Physical Review Letters* **101**, 016403 (2008). Laboratory Directed Research and Development funds the work.

Contact: Tomasz Durakiewicz

Nanoengineered microstructures for tunable high-current, HTS wires

A recent paper published in *Advanced Materials* reported significant progress in performance of high temperature superconducting (HTS) wire made by a commercially scalable method. The lead author, Terry Holesinger (MPA-STC), is also the principal investigator on the MPA-STC–American Superconductor Cooperative Research and Development Agreement focused on high temperature superconducting wire development. Additional MPA-STC authors included Leonardo Civale, Boris Maiorov, Matt Feldmann and Yates Coulter. The work included collaborators from American Superconductor Corporation, Argonne National Laboratory, Oak Ridge National Laboratory, and the National High Magnetic Field Laboratory in Tallahassee, Flordia. Reference: "Progress in Nanoengineered Microstructures for Tunable High-Current, High-Temperature Superconducting Wires," *Advanced Materials* **20**, 391-407 (2008).



▲ *Schematic of a coated high temperature superconducting wire.*

In high temperature superconducting wire, high critical current densities in thick films of YBaCuO superconductor depend upon the types of engineered nanoscale defects and their densities within the film, which cause flux pinning. Applications such as cable, motors, and generators require the presence of flux pinning defects to maintain substantial critical current densities in applied fields. Cables operate in low magnetic fields, while motors and generators experience higher field conditions. Therefore tuning the flux pinning characteristics of the wires to have optimal function for the actual operating conditions is needed. In addition, the YBaCuO coated conductors must be homogeneous on the macroscale in the length and breadth of the wire. The scientists demonstrated advances in high-performance YBCO coated conductors using chemical solution deposition and the subsequent processing to nanoengineer the microstructure for tunable superconducting wires by methods suitable for large-scale manufacturing. This work shows substantial improvements in the understanding of flux pinning behavior in high temperature superconducting films, as well as methods of controlling the flux pinning in a commercially viable processing method. DOE's Office of Electricity Delivery and Energy Reliability funded the work.

Nano50 award for directed assembly of nanowire contacts

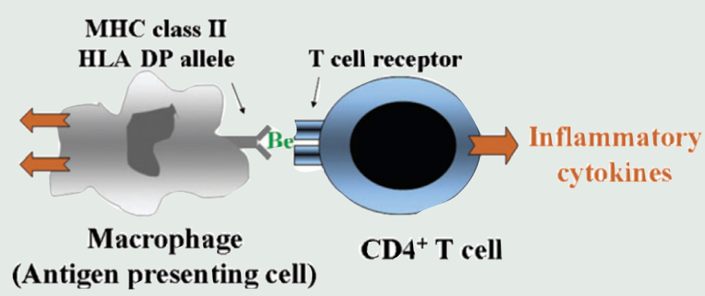
Tom Picraux (MPA-CINT) and collaborators from Arizona State University and CINT at Sandia National Laboratories discovered a more efficient way of fusing charge-carrying electrical contacts to "nanowires" of silicon to create the nanotechnology needed for future advances in modern electronics, sensing, and energy collection. *Nanotech Briefs* selected this work, published in *Applied Physics Letters* and featured on the cover of the journal, to receive one of the 2008 Nano 50 Awards that recognize "the top 50 technologies, products, and innovators that have significantly impacted, or will impact, the development of nanotechnology."

The difficulty and cost of forming critical metal-silicon junctions have hindered large-scale fabrication required for applications in which nanowires must be integrated into systems, such as sensor arrays or solar cells. Current nanomanufacturing relies on ultra-high resolution patterns to accurately fabricate the connections between metal contacts. Electron beam lithography is used to connect the metal contacts to each nanowire. This process, in which the wire pattern is "written" with a beam of electrons to one nanowire at a time, is much too slow for practical application. To meet this challenge, the researchers designed a method that eliminates the final lithography step. The team used lithography initially to create a set of gold electrodes. They then utilized an alternating electric field in a technique called dielectrophoresis to pull the silicon nanowires from a solution into place between the electrodes. In the subsequent electrodeposition process, the researchers selectively deposited nickel only where the underlying gold electrodes were located. After the silicon nanowires were completely covered, they were heated to several hundred degrees Celsius to establish good contacts. With this "directed assembly" approach, the electric field guides the simultaneous creation of all the contacts in the correct location at once. Electrodeposition is routinely used in the semiconductor industry for on-chip interconnects and for printed-circuit boards; thus this method may be extendable to nanowire contact assembly.

The research addresses a need for the directed assembly of electrical contacts of nanowires, an important step in the integration of nanowires into electronic, photonic, and sensing systems. This method may also have larger-scale applications, including biological and chemical sensor networks and the fabrication of nanowire solar cells. The team will receive the award at the NASA Tech Briefs National Nano Engineering Conference held next month in Boston.

Multidisciplinary research on CBD focus of invited article

Chronic beryllium disease (CBD) is a debilitating, incurable, and often fatal disease caused by the inhalation of beryllium particulates. CBD can be triggered by very low beryllium exposures (<2.0 μg m-3) and the delay of symptoms can vary from 1 to more than 20 years. The growing use of beryllium, in products ranging from computers to dental prosthetics, necessitates a molecular based understanding of the disease in order to prevent and cure CBD. For example, 390 tons of beryllium was used in the U.S. in 2000.



Mechanism of chronic beryllium disease initiation. A beryllium antigen (center) binds to an HLA molecule on an antigen presenting cell and is presented to a T cell, triggering the immune response that results in chronic beryllium disease.

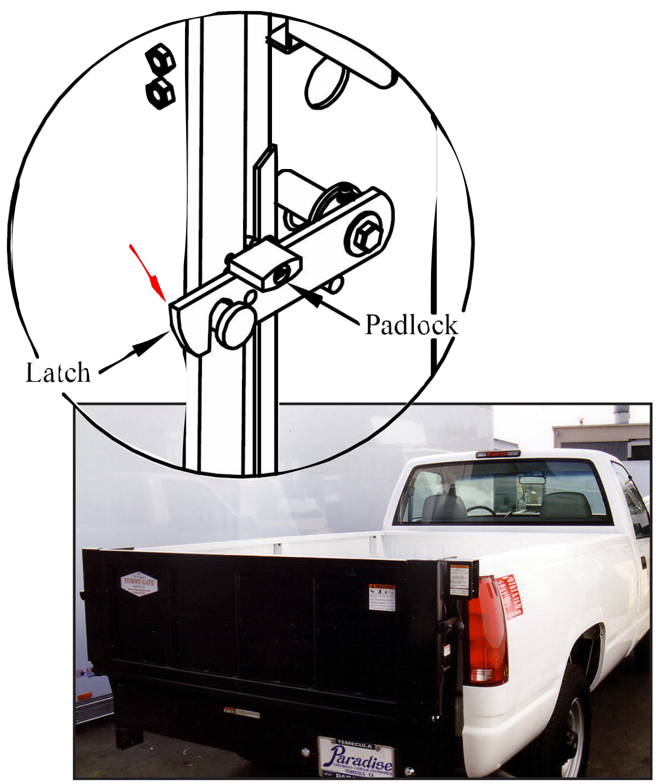
Brian L. Scott and Mark McCleskey (both MPA-MC), Anu Chaudhary and Elizabeth Hong-Geller (both B-7), and S. Gnanakaran (T-10) investigated the molecular basis of CBD during the past six years, employing a multidisciplinary approach of bioinorganic chemistry and immunology. They published the results of this work, including beryllium speciation, inhalation and dissolution, and immunology, in an invited feature article in *Chemical Communications* 2837-2847 (2008).

Beryllium inhaled into the lungs is detected by antigen presenting cells. An unknown beryllium species serves as the antigen. The antigen is created when beryllium interacts with a specific peptide or protein in the body. The immune response to beryllium is triggered when the beryllium antigen is bound to a human leukocyte antigen (HLA) molecule, and presented to a T lymphocyte (T cell). CBD is marked by hyperproliferation of CD4+ T cells. This is the basis for the lymphocyte proliferation test, currently used for diagnosis of sensitization or disease. Research with model complexes demonstrates that beryllium prefers to bind in specific sites, through the displacement of an H+ in a strong hydrogen bond. This new paradigm of beryllium binding can be used in future studies as a model for beryllium binding in proteins. Experimental evidence of approximately six beryllium atoms in the HLA-DP binding groove is consistent with earlier theoretical studies. Two consecutive LDRD-DRs funded the work. The principal investigator of the first DR was Nan Sauer and the second was Tom McCleskey. The work is highlighted in *Chemical Biology*, www.rsc.org/Publishing/Journals/CB/Index.asp.

HeadsUP!

Vehicle lift gate latch causes cut to worker;
Groups encouraged in inspect trucks

The MPA WSST found that an MPA worker recently cut his elbow on a lift gate latch on the back of a pick-up (see photo at right) at the NHMFL. The cut was not serious, but did require stitches. While carrying a box, the worker was walking from the driver's side to the back. As he rounded the corner of the truck, he hit his left elbow on the latch. The tip of the latch is the furthest protruding object from the gate assembly. It was found that the latch was sharp at the point shown by the red arrow (see illustration). The worker went to Occupational Medicine to get stitches and a tetanus shot. A co-worker ground down the sharp corner on both latches to greatly reduce the chance of this happening again.



Groups are asked to inspect their vehicles with lift gates and grind/file the corner if needed. The process is easy and should only take 5-10 minutes per truck.

Magnetic resonance force microscopy featured on journal cover

LANL magnetic resonance force microscopy research is featured on the August 8 cover of *Physica Status Solidi A*. The work involves a collaboration between MPA-10 (Evgueni Nazaretiski, Kevin Graham and Roman Movshovich), T-11 (Ivar Martin), CINT (Elshan Akhadov), and Ohio State University (C. Hammel and D. Pelekhov).

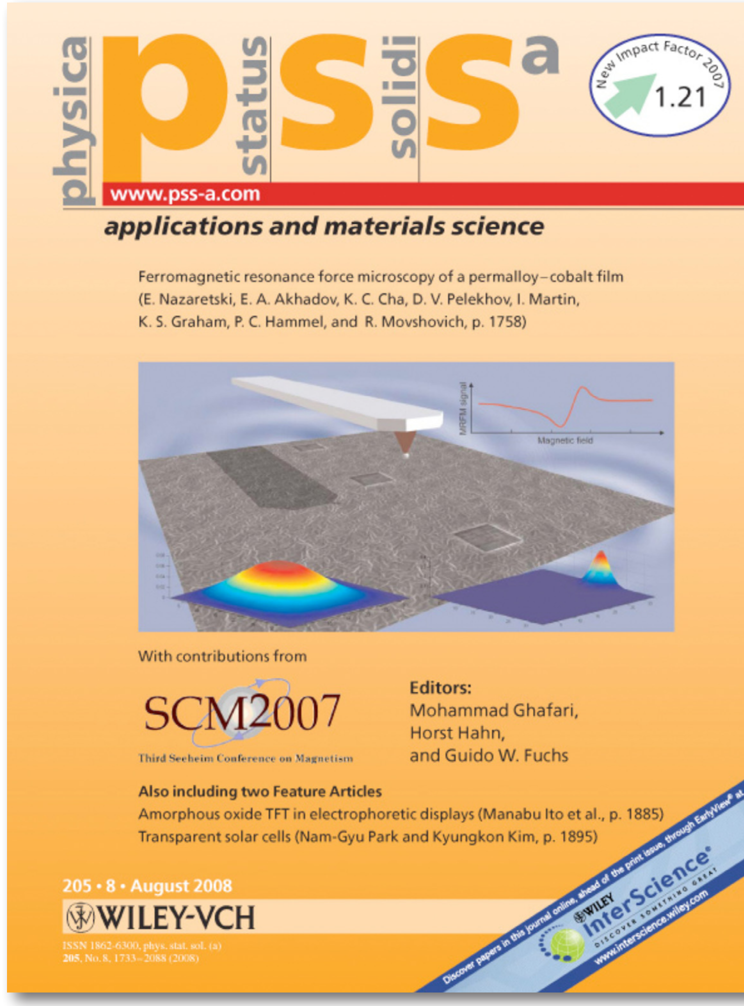
Magnetic resonance force microscopy (MRFM) offers a means of performing local ferromagnetic resonance unavailable through conventional resonance techniques. The authors studied the evolution of the MRFM force spectra in a continuous 20 nm thick cobalt–permalloy film as a function of lateral position. They observed localized resonance signals originating from cobalt and permalloy.

The spatial resolution in the experiments was determined to be better than a few microns, thus demonstrating the possibility of performing localized spectroscopic studies in continuous ferromagnetic media. These types of measurements enable detection of impurities and imperfections in magnetic films.

The journal cover picture illustrates the MRFM experiments. The cantilever is equipped with a micromagnetic tip to generate the field gradient and couple to the in-resonance spins of the sample. In the case of a ferromagnetic sample, the inhomogeneous probe field excites highly localized ferromagnetic resonance modes.

The typical MRFM signal is shown in the upper right corner. The positive contribution corresponds to the bulk-like resonance signal similar to those observed in conventional magnetic resonance experiments. The negative part of the signal represents the tip-induced resonance with the high degree of localization. Varying the probe-sample distance changes the localization of the ferromagnetic resonance from hundreds of micrometers down to sub-micron range. Two panels on the bottom demonstrate the numerically simulated lowest frequency resonance modes and their spatial confinement.

Laboratory Directed Research and Development and CINT funded the work. Reference, "Ferromagnetic Resonance Force Microscopy Studies of a Continuous Permalloy-Cobalt Film," *Physica Status Solidi A* **205**, 1758-1761 (2008).



The researchers' measurements enable detection of impurities and imperfections in magnetic films.

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www.lanl.gov/orgs/mpa/materialsmatter.shtml.

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